N-Phenethyl O-propyl thiocarbamate

Inchi: InChI=1S/C12H17NOS/c1-2-10-14-12(15)13-9-8-11-6-4-3-5-7-11/h3-7H,2,8-10H2,1H3,(H
InchiKey: SROGOSNHDATCGM-UHFFFAOYSA-N
Formula: C12H17NOS
SMILES: CCCOC(=S)NCCc1ccccc1
Mol. weight [g/mol]: 223.33

Physical Properties

Property code	Value	Unit	Source
gf	264.02	kJ/mol	Joback Method
hf	13.27	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.530		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
ripol	2929.00		NIST Webbook
tb	643.27	K	Joback Method
tc	863.22	K	Joback Method
tf	360.58	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.78	J/mol×K	643.27	Joback Method
cpg	475.54	J/mol×K	679.93	Joback Method
cpg	489.32	J/mol×K	716.59	Joback Method
cpg	502.20	J/mol×K	753.25	Joback Method
cpg	514.24	J/mol×K	789.90	Joback Method
cpg	525.50	J/mol×K	826.56	Joback Method
cpg	536.04	J/mol×K	863.22	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R440058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume